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Ensuring reliability, reproducibility and transferability in atomistic simulations: The knowledgebase of interatomic models (https://openkim.org)

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ABSTRACT

Atomistic simulations using empirical interatomic potentials play a key role in realistic scientific and industrial applications. This discussion describes an NSF-funded effort to develop an open-source online tool for promoting the use and reliability of interatomic models. The Knowledgebase of Interatomic Models (https://openkim.org) allows users to compare model predictions with reference data, to generate new predictions by uploading simulation test codes, and to download models conforming to an application programming interface (API) standard that has been developed in collaboration with the atomistic simulation community. An overview will be given of the KIM project and its main components which include the KIM API, the KIM data structure for representing arbitrary material properties, the KIM processing pipeline, and the KIM visualization framework.